

”One-dimensional” Coherent States and Oscillation Effects in Metals in a Magnetic Field

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The ”one-dimensional” coherent states are applied to describe such macroscopic quantum phenomena as the Shubnikov - de Haas and the de Haas-van Alphen oscillation effects in metals, semimetals, and degenerate semiconductors. The oscillatory part of the electron density of states in a magnetic field is calculated. A substantial simplification of calculations is achieved.

I. INTRODUCTION

R. J. Glauber [1,2] introduced in 1963 the concept of a coherent state $|\alpha\rangle$ as an eigenstate of a non-hermitian annihilation operator \hat{a} of excitations of the boson type ($\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$). The Schrödinger equation for a charge in a constant uniform magnetic field reduces to the Schrödinger equation for a one-dimensional displaced harmonic oscillator. The use of coherent states significantly simplifies mathematical calculations of the oscillating part of the thermodynamic characteristics. Coherent states are eigenstates of a non-hermitian operator and are not orthogonal, i.e. transitions between different coherent states can occur spontaneously. The Shubnikov-de Haas and de Haas-van Alphen effects are not only quantum effects. They are also macroscopic effects, and in these respects (the quantum character and macroscopic scale, simultaneously) they are related with such phenomena as superconductivity, weak-link superconductivity (Josephson effects), laser radiation, and von Klitzing’s effect (the quantum Hall effect). Our aim is to demonstrate clearly (by using the method of coherent states combined with an universal approach to the thermodynamic and kinetic effects in metals in a constant uniform magnetic field) not only the mathematical advantage of such a combination, but also to establish the physical reasons for why the mathematical description is adequate for the physics of the quantum oscillation effects. The physical nature of oscillations of the kinetic coefficients of a metal in a magnetic field (Shubnikov-de Haas effect) as well as oscillations of the thermodynamic potentials and their derivatives has been established on the basis of Landau’s theory of diamagnetism. The oscillations are governed by two factors: the presence of the Fermi surface and the radical change in the density of states $\rho(\varepsilon)$ when the magnetic field is turned on [3]. Turning on a constant uniform magnetic field \mathbf{H} parallel to the z-axis makes the motion of a current-carrying

particle quasi-one dimensional and the density of states changes from $\rho_{3d}(\varepsilon) \propto \sqrt{\varepsilon}$ to $\rho_{1d}(\varepsilon) \propto \frac{1}{\sqrt{\varepsilon}}$ (for the three- and one-dimensional systems, respectively). Due to the Landau quantization of the electron energy spectrum this inverse square-root singularity of $\rho(\varepsilon)$ is repeated many times in the energy interval $0 \leq \varepsilon \leq \mu$ (μ is the chemical potential), when the condition $\mu \gg \hbar\omega_H$ is satisfied (where $\omega_H = eH/mc$ is the cyclotron frequency; m, e is the effective mass and the charge of the current carrier, respectively, and c is the light velocity in vacuum. For energies $\varepsilon \approx \mu$ near the Fermi surface the density of states $\rho(\varepsilon)$ is an almost-periodic function of the magnetic field. This is the origin for the oscillatory character of the magnetic field dependence of both the thermodynamic quantities (”linear” with respect to $\rho(\varepsilon)$) and the kinetic coefficients (”quadratic” with respect to $\rho(\varepsilon)$). The oscillation period is the same for both types of quantities and is equal to the oscillation period of the function $\rho(\varepsilon)$.

II. SOME THERMODYNAMICS RELATIONS

The thermodynamic potential $\Omega_H = F_H - \mu N$ is defined by the expression [4]

$$\Omega_H = -T \sum_{\nu} \ln \left[1 + e^{(\mu - \varepsilon_{\nu})/T} \right]. \quad (1)$$

In the integral form it may be written as

$$\Omega_H = -T \int_0^{\infty} d\varepsilon \rho(\varepsilon) \ln \left[1 + e^{(\mu - \varepsilon)/T} \right]. \quad (2)$$

The density of states $\rho(\varepsilon)$ is given by

$$\rho(\varepsilon) = \sum_{\nu} \delta(\varepsilon - \varepsilon_{\nu}) = Tr \delta(\varepsilon - \hat{\mathcal{H}}), \quad (3)$$

where F_H is the free energy, N is the total number of particles, T is the temperature (in energy units), ν is the

set of all the quantum numbers characterizing a single-particle state and $\hat{\mathcal{H}}$ is the single particle Hamiltonian. For the thermodynamic potential derivatives we have

$$N = -\left(\frac{\partial \Omega_H}{\partial \mu}\right)_{T,V,H}, \quad M = -\left(\frac{\partial \Omega_H}{\partial H}\right)_{T,V,\mu},$$

$$C = -T\left(\frac{\partial^2 \Omega}{\partial T^2}\right)_{V,\mu,H}, \quad (4)$$

where M is the magnetic moment and C is the heat capacity. We shall calculate the density of states from Eq.(2), setting $T = 0$ for simplicity. Then the $\rho(\varepsilon)$ transforms into $\rho(\mu)$ and is related with Ω_H by the expression

$$\rho(\mu) = -\left(\frac{\partial^2 \Omega_H}{\partial \mu^2}\right)_{V,H,T=0}. \quad (5)$$

We can easily see from Eq.(5), the density of states $\rho(\mu)$ at the Fermi surface is not only related with the observable quantities presented in Eq.(4). Its oscillatory part $\tilde{\rho}(\mu)$ contains the period of the oscillations, which in turn through the Lifshitz-Onsager relation determines the area of the extremal sections of the Fermi surface by a plane perpendicular to \mathbf{H} . The oscillatory part $\tilde{\rho}(\varepsilon)$ of the density of states also answers the question about the physical nature of the oscillations of the kinetic coefficients in a magnetic field. As is well known from the theory of the Shubnikov-de Haas effect, the appearance of a nonzero current in the direction of the electric field $\mathbf{E}||\mathbf{x}$ is attributable to the appearance of electron scattering, which under the conditions of the Shubnikov-de Haas effect can be assumed to be elastic [3, 5]. The fact that $\rho(\varepsilon)$ in Eq.(3) is represented in the form of a trace makes it possible to employ any complete set of wave functions in the computational procedure. Oscillatory wave functions (which are eigenfunctions of the number operator of boson excitation $\hat{a}^\dagger \hat{a}|n\rangle = n|n\rangle$) do not carry any information about the presence of the Fermi surface, while for the coherent states $|\alpha\rangle$ (which are eigenfunctions of the operator $\hat{a}(\hat{a}|\alpha\rangle = \alpha|\alpha\rangle)$) the average number of the particles is equal to

$$\langle \alpha | \hat{a}^\dagger \hat{a} | \alpha \rangle = \bar{n}_\alpha \simeq \frac{\mu}{\hbar \omega_H}. \quad (6)$$

In addition, the coherent states are characterized by a well-defined phase [2,6]. This is related with the existence of a phase characteristic(cyclotron period) of the oscillation phenomena under study. It suggests us to use coherent states for our problem.

III. COHERENT STATES OF A CHARGED PARTICLE IN A CONSTANT UNIFORM MAGNETIC FIELD

Coherent states appear when one solves a task for an linear oscillator. Some physical phenomena (supercon-

ductivity, Shubnikov - de Haas, de Haas-van Alphen effects) are quantum in their physical nature and macroscopical in their scale. Macroscopic scale indicates on a possibility of an almost classical description of such phenomena. The coherent states are much more convenient to describe simultaneously a field phase and amplitude, and to show a connection between the classical and quantum field description. Historically, L. D. Landau was the first to show that the Schrödinger equation for the eigenfunctions and eigenvalues of a charge in a constant magnetic field has the form of the Schrödinger equation for the one-dimensional linear oscillator. Coherent states have been used to recast in new terms the theory of Landau dimagnetism and the theory of the de Haas-van Alphen effects for free electron gas.

The achievements of the physics of coherent states have not been extended enough to oscillation effects in metals with an arbitrary dispersion relation for electrons or to numerous other quantum physical phenomena observed in metals in a magnetic field.

We will introduce the coherent states for a charge in a constant magnetic field $\mathbf{H}||\mathbf{z}$ and the Hamiltonian [7]

$$\hat{\mathcal{H}} = \frac{1}{2m}(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A})^2 + \hat{\mathcal{H}}_\sigma = \hat{\mathcal{H}}_\perp + \hat{\mathcal{H}}_\mathbf{z} + \hat{\mathcal{H}}_\sigma, \quad (7)$$

$$\hat{\mathcal{H}}_\mathbf{z} = \frac{\hat{p}_z^2}{2m}, \quad \hat{\mathcal{H}}_\sigma = -\frac{g}{2}\mu_B\sigma_z H, \quad \sigma_z = \pm 1, \quad (8)$$

where $\hat{\mathbf{p}}$ is the momentum operator, m is the bare electron mass, g^* is the effective spectroscopic splitting factor, μ_B is the Bohr magneton.

We choose the vector potential \mathbf{A} of the magnetic field in the Landau-gauging [7] as follows

$$\mathbf{A} = \mathbf{A}(-yH, 0, 0), \quad \mathbf{H} = \nabla \times \mathbf{A}. \quad (9)$$

In this case $\hat{\mathcal{H}}_\perp$ corresponds to an one-dimensional oscillator along the y axes

$$\hat{\mathcal{H}}_\perp = \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega_H^2(y - y_0)^2 \quad (10)$$

(where $y_0 = -cp_x/eH$) instead of two coupled oscillators in gauging $\mathbf{A} = (1/2)[\mathbf{H}\mathbf{r}]$. It gives us a possibility to avoid using of "two-dimensional" coherent states (see [8]). In dimensionless coordinates

$$\eta = \frac{y - y_0}{l_H}, \quad l_H = \left(\frac{\hbar}{m\omega_H}\right)^{1/2}, \quad (11)$$

the Hamiltonian $\hat{\mathcal{H}}_\perp$ takes the form

$$\hat{\mathcal{H}}_\perp = \frac{1}{2}\hbar\omega_H(\hat{p}_\eta^2 + \eta^2), \quad (12)$$

$\hat{p}_\eta = -i\nabla_\eta$. We introduce the operators \hat{a} and \hat{a}^+

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\eta + \frac{\partial}{\partial \eta} \right), \quad \hat{a}^+ = \frac{1}{\sqrt{2}} \left(\eta - \frac{\partial}{\partial \eta} \right) \quad (13)$$

$[\hat{a}, \hat{a}^+] = 1$. Then \hat{H}_\perp results in

$$\hat{H}_\perp = \hbar \omega_H \left(\hat{a}^+ \hat{a} + \frac{1}{2} \right), \quad (14)$$

and

$$\hat{H} = \hbar \omega_H \left(\hat{a}^+ \hat{a} + \frac{1}{2} \right) + \frac{\hat{p}_z^2}{2m} - \frac{g^*}{2} \mu_B \sigma_B H. \quad (15)$$

Thus, the partial motion of an electron in a magnetic field in the xy plane is described by the Eq. (14), which contains the operators \hat{a} , \hat{a}^+ (defined in Eq.(13)), satisfying the Bose commutation relations. With the help of the operators \hat{a} , \hat{a}^+ we determine the states:

- a) the vacuum state $|0\rangle$ such that $\hat{a}|0\rangle = 0$;
- b) the Fock (after V.A.Fock) state $|n\rangle$, which is an eigenstate of the operator $\hat{n} = \hat{a}^+ \hat{a}$;

$$\hat{n}|n\rangle = n|n\rangle, \quad |n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle; \quad (16)$$

c)the one-dimensional coherent state $|\alpha\rangle$ which is an eigenstate of the operator \hat{a}

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle. \quad (17)$$

The coherent state $|\alpha\rangle$ can be obtained also with the help of the displacement operator $\hat{D}(\alpha)$

$$|\alpha\rangle = \hat{D}(\alpha)|0\rangle, \quad (18)$$

where

$$\hat{D}(\alpha) = e^{\alpha \hat{a}^+ - \alpha^* \hat{a}} = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^+} e^{-\alpha^* \hat{a}}. \quad (19)$$

Thus, we have a complete normalized set of wave functions, which are the eigenfunctions of non-hermitian operator and for this reason are not orthogonal.

It should be specially noted, however, that the partial motion of a fermion (electron) in the xy plane in the magnetic field \mathbf{H} is described with the help of a boson field.

IV. OSCILLATIONS OF THE ELECTRON DENSITY OF STATES

We can employ the following complete normalized set of wave functions to calculate $\rho(\mu)$ of a metal in a quantizing magnetic field

$$|\sigma_z, p_z; \alpha\rangle = L_z^{-1/2} e^{(ip_z z/\hbar)} \chi|\alpha\rangle, \quad (20)$$

where

$$\hat{\sigma}_z \chi = \sigma_z \chi, \quad \sigma_z = \pm 1, \quad (21)$$

L_z is the normalization length, and $\hat{\sigma}_z$ is the Pauli matrix.

Taking the trace in Eq. (3) and using Eq. (20), we obtain

$$\begin{aligned} \rho(\mu) &= \sum_{p_z, \sigma_z} \int \frac{d^2 \alpha}{\pi} \langle \alpha; P_z, \sigma_z | \delta(\mu - H) | \sigma_z, p_z; \alpha \rangle \\ &= \frac{L_z}{\pi(2\pi\hbar)^2} \sum_{\sigma_z} \int_{-\infty}^{\infty} dp_z \int d^2 \alpha \int_{-\infty}^{\infty} dt \\ &\quad \times \langle \alpha; p_z, \sigma_z | e^{i(\mu - \hat{H})t/\hbar} | \sigma_z, p_z; \alpha \rangle, \end{aligned} \quad (22)$$

where $d^2 \alpha = d(Re \alpha) d(Im \alpha)$. In the operator \hat{H} all three terms commute one with another. We obtain the following relations:

$$\sum_{\sigma_z=\pm 1} e^{i(t/\hbar)(g^*/2)\mu_B H} = 2 \cos \left(\frac{g^* \mu_B H}{2\hbar} t \right); \quad (23)$$

$$\int_{-\infty}^{\infty} dp_z e^{-\frac{itp_z^2}{2m\hbar}} = \left(\frac{2\pi\hbar m}{|t|} \right)^{1/2} e^{-i\frac{\pi}{4} \text{sign } t}; \quad (24)$$

$$\begin{aligned} \langle \alpha | e^{-it\omega_H \hat{a}^+ \hat{a}} | \alpha \rangle &= \sum_{n=0}^{\infty} \langle \alpha | e^{-it\omega_H \hat{a}^+ \hat{a}} | n \rangle \langle n | \alpha \rangle \\ &= \sum_{n=0}^{\infty} e^{-it\omega_H n} |\langle n | \alpha \rangle|^2 = e^{-|\alpha|^2(1 - e^{-it\omega_H})}. \end{aligned} \quad (25)$$

In the last equation we have used the condition

$$\sum_{n=0}^{\infty} |n\rangle \langle n| = 1 \quad (26)$$

of the completeness of the set of the Fock states. The result for the scalar product of the Fock and coherent states is as follows

$$\begin{aligned} \langle n | \alpha \rangle &= \left\langle n \left| e^{-|\alpha|^2/2} e^{\alpha \hat{a}^+} \right| 0 \right\rangle \\ &= \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2}. \end{aligned} \quad (27)$$

The density of states $\rho(\mu)$ at the Fermi surface results in the form of a single integral

$$\begin{aligned} \rho(\mu) &= \frac{L_z \Phi m^{1/2}}{(2\pi\hbar)^{3/2} \Phi_0} \int_{-\infty}^{\infty} dt \frac{e^{i(\frac{\mu t}{\hbar} - \frac{\pi}{4} \text{sign } t)} \cos \left(\frac{g^* \mu_B H}{2\hbar} t \right)}{i|t|^{1/2} \sin(t\omega_l)}, \\ \Phi &= L_x L_y H, \quad \Phi_0 = \frac{ch}{e}. \end{aligned} \quad (28)$$

It is calculated with the help of the residue theorem by integrating along the contour shown in Fig. 1.

The oscillating part of the density of states $\tilde{\rho}(\mu)$ is determined by the contribution into the integral of the poles located on the real axis at the points

$$t_k = \frac{2\pi}{\omega_H} K, \quad K = \pm 1, \pm 2, \pm 3, \dots \quad (29)$$

and has the form

$$\begin{aligned} \tilde{\rho}(\mu) &= \frac{mV}{\pi^2 \hbar^2} \left(\frac{eH}{c\hbar} \right)^{1/2} \sum_{K=1}^{\infty} K^{-1/2} \\ &\times \cos \left(\frac{\pi g^* m}{2m_0} K \right) \cos \left(2\pi K \frac{\mu}{\hbar\omega_H} - \frac{\pi}{4} \right), \end{aligned} \quad (30)$$

which contains a period of the oscillations

$$\Delta \left(\frac{1}{H} \right) = \frac{e\hbar}{mc\mu}. \quad (31)$$

V. DISCUSSION

Our approach to the analysis of oscillation effects in a metal in a magnetic field makes it possible not only to substantially simplify the mathematical procedure as compared with the traditional method of analyzing these phenomena, but also to study in a universal manner both the thermodynamics and kinetic effects, to easily extend the analysis to the case of current carriers with an arbitrary energy spectrum and nonzero temperature, and to include the effect of scattering on the form of the oscillation dependence.

The physical reason for the simplification achieved in the mathematical procedure is that the coherent state employed in the calculations describe quantum macroscopic and therefore also quasi-classical phenomena, which are the Shubnikov-de Haas and de Haas-van Alphen effects in metals, semimetals and degenerate semiconductors.

VI. ACKNOWLEDGEMENTS

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FIG. 1. The integration contour in the complex plane t for the calculation of the integral Eq. (28).

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